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ABSTRACT

The Hydrogen-Oxygen Regenerative Fuel Cell System has been identified as a key component for energy storage in support of future lunar missions. Since the H_2-O_2 regenerative electrochemical conversion technology has not yet been tested in space applications, it is necessary to implement predictive techniques to develop initial feasible system designs. The ASPEN simulation software furnishes a constructive medium for analyzing and for optimizing such systems. A rudimentary regenerative fuel cell system design has been examined using the ASPEN simulator and this modular approach allows for easy addition of supplementary ancillary components and easy integration with life support systems. The modules included in the preliminary analyses may serve as the fundamental structure for more complicated energy storage systems.

INTRODUCTION

The Planetary surface power program is a key element of the Space Exploration Initiative (SEI) instituted at the National Aeronautics and Space Administration. Regenerative fuel cell systems (RFCS) can facilitate photovoltaic energy storage for operations on the Lunar and Martian surfaces. The fuel cell subsection of the RFCS will consume hydrogen and oxygen to produce electricity and water when solar energy is not available. During the sunlit portion of the orbit cycle, photovoltaic arrays will supply power to the electrolyzer subsection of the RFCS where water will be electrochemically converted to hydrogen and oxygen. A feasible RFCS for Lunar and Martian applications must operate at high efficiencies for relatively long time periods.

Design goals for Lunar and Martian RFCS are a 25 kWe supply operating for 20,000 hours in an autonomous mode. Alkaline electrolyte systems and Proton Exchange Membranes (PEM) are the two options being considered for the electrochemical converters, providing four separate options for the entire RFCS : an all alkaline system, an all PEM system, and two different hybrid alkaline/PEM

systems. Since each possible configuration cannot be extensively tested due to time and resource limitations, predictive techniques must be implemented to guide the RFCS design.

An assortment of PEM and alkaline RFCS conceptual designs and simulation efforts have been completed to date but limited experimental data exist. Van Dine et al. [1] examined various RFCS configurations for geosynchronous satellite missions while Hoberecht, et al. [2] modeled the performance of a 10 kW alkaline RFCS for applications in Low Earth Orbit. The SAREF simulation program developed at Dornier [3] contains transient capabilities and includes thermal control analyses. McElroy [4] demonstrated long term PEM fuel cell (40,000 hrs of 4 cell stack at 120 A/sq.ft.) and electrolyzer (near 100,000 hrs.) operation and analyzed a RFCS utilizing PEM technology for Lunar and Martian surface power. Saucier [5] reported successful operation of an experimental hybrid system (alkaline fuel cell and PEM electrolyzer) using Low Earth Orbit time durations (fuel cell operation for 36 minutes, electrolyzer operation for 54 minutes) and Martin reported on the experimental results for operating an integrated, all alkaline regenerative fuel cell [6]. The present effort focused strictly upon the computer simulation of a 25 kWe RFCS for energy storage on the Lunar and Martian surfaces.

OBJECTIVES

The objective of the present effort was to develop a modular computer simulation framework to predict performance characteristics of a 25 kW RFCS. A modular framework was demanded so that alkaline and/or PEM technology with all associated ancillary components could be readily interchanged within the RFCS flowsheet. The modular approach allows for easy analyses of assorted RFCS configurations and subsequent design optimization.

APPROACH/BACKGROUND

Regenerative fuel cell energy storage system performance characteristics were simulated using

ASPEN PLUS (Trademark of Aspen Technology, Inc.) because ASPEN PLUS afforded a modular programming environment with a data bank suitable for characterizing the thermodynamic conditions of the fuel cell reactants and products. A disadvantage of this approach was that the transient performance of the electrochemical system (during start-up and shut-down) could not be estimated without significant modifications. Consequently, only steady-state RFCS performance was predicted in this study.

While effects of the ancillary equipment (pumps, compressors, heat exchangers, etc.) could be analyzed quite readily using the ASPEN PLUS simulator, the fuel cell and electrolyzer module analyses required detailed specifications from the user. Regenhardt [7] devised an ASPEN fuel cell block to simulate behavior of solid oxide, molten carbonate, and phosphoric acid fuel cells for terrestrial applications but alkaline and PEM fuel cell systems for space applications were not simulated. In the present study, Fortran blocks were coded to facilitate transfer of the essential fuel cell and electrolyzer information to and from the ASPEN Flowsheet. For example, heat duties for the fuel cell and electrolyzer modules that were computed within the ASPEN simulator were modified to account for (IR) heat generation in the electrolyte and the fuel cell and electrolyzer voltages were estimated from the correlations used by Lu [8]. All vapor phase thermodynamic properties were estimated using the Redlich-Kwong cubic equation of state and Henry's Law was applied when appropriate.

RESULTS

The fuel cell subsection of the RFCS flowsheet, depicted in Figure 1, is similar to that assumed by Hoberecht, et al. Inlet fuel cell oxidant gas is dead-ended whereas product water was removed and condensed from the anode gas stream. Makeup hydrogen gas was blended with the exiting anode gas stream before the water was condensed; therefore, it was desirable to maintain a relatively cold H₂ storage temperature. A recirculating hydrogen pump/water separator served to remove the water and to maintain the desired anode gas flow rate. A post-condenser water trap, an anode gas stream pre-heater, as well as heat exchangers to control the makeup reactant gas temperatures were added to complete the flowsheet in Figure 1. The temperature of the anode gas exiting the fuel cell was maintained constant by cooling the fuel cell stack during simulated operation. Initial parametric studies focused upon the effects that the hydrogen gas utilization ratio and the fuel cell operating conditions had upon thermal requirements of the fuel cell subsection. These elementary analyses excluded transient thermal management issues that are the topic of a separate study, such as the temperature changes that occur within the reactant gas storage tanks during operation. Similarly, ancillary RFCS components were embodied in the system flowsheet. The influences of those components on overall system performance were

neglected, except for the small (roughly 2 K) temperature increase imparted to the hydrogen loop caused by inefficient pump operation.

Operating conditions for the alkaline fuel cell stacks were fixed to those values given in Table I, unless otherwise noted. Those operating conditions for Lunar operations differed from the current density (366 mA/sq.cm.) and charge/discharge time ratio (22.8/1.2) assumed for the 25 kW RFCS analyzed by Van Dine, et al. for satellites in GEO orbit. The thermodynamic phase of the anode gas stream which exited the fuel cell depended upon the temperature, pressure, and composition of that stream. For a specified fuel cell operating pressure, the relationship between the fuel utilization ratio (FUR) and the minimum fuel cell exit temperature was that represented by Figure 2. The FUR was defined as the [H₂ gas flow rate into the fuel cell minus the H₂ gas flow rate out of the fuel cell] divided by the H₂ gas flow rate into the fuel cell. Feasible FUR values were those which mandated an all vapor fuel cell exit stream. Note that for a designated FUR, the feasible range for the fuel cell exit temperature was that portion above the curve in Figure 2. The FUR affected the total fuel cell and condenser cooling requirements in the manner shown in Figure 3. Larger FUR values relieved the cooling duty of the condenser but increased the cooling duty for the fuel cell. Total cooling requirements increased at very low FUR values since the large amount of unreacted hydrogen was continually cooled and heated. Specific water removal techniques for fuel cell operation were discussed by Kordes, et al. [9] and the steady state nature of this simulation implied that the amount of water removed from the fuel cell stack was equal to the amount of water produced by the overall fuel cell reaction.

The electrolysis subsection of the RFCS, depicted in Figure 4, is similar to those subsections reported by Van Dine et al. and by Hoberecht et al. An inlet water heat exchanger and feed pump were added to the system along with product hydrogen and oxygen driers. Operating conditions for the electrolyzer units were those outlined in Table II unless otherwise stated. Note that the electrolyzer current density was much larger for the Lunar application than that used for the RFCS study (20 mA/sq.cm.) for satellite purposes [1].

Since the electrolyzer operates during the sunlit portion of the orbit cycle, it would be practical to supply heat to the electrolyzer stack to increase the operating efficiency. The thermoneutral electrolyzer efficiency increased with higher electrolyzer exit temperatures in the manner represented in Figure 5. In Figure 6, the electrolyzer heat duties needed to achieve those electrolyzer exit temperatures are shown. In both Figure 5 and Figure 6, the total current was assumed to be constant.

The entire flowsheet could be easily modified to include more components or to exclude some

components, and to redirect reactant or product streams to improve thermal management. These issues will be investigated in future design optimization studies. An important issue for Lunar and Martian surface power applications of RFCS is the operational lifetime of the RFCS. Electrolyte concentration, operating temperature and pressure, and electrochemical converter efficiency are all inter-related. Each influences the lifetime of the fuel cell and electrolyzer stacks. The RFCS operating parameters can be changed to optimize the lifetime, system mass, system volume, or cost.

CONCLUSIONS

Since the H_2-O_2 regenerative electrochemical conversion technology has not yet been tested in space applications, it is necessary to implement predictive techniques to develop initial feasible system designs. The ASPEN simulation software furnishes a constructive medium for analyzing and for optimizing such systems. A rudimentary regenerative fuel cell system design has been examined using the ASPEN simulator. This modular approach allows for easy addition of supplementary ancillary components and easy integration with life support systems. The modules included in the preliminary analyses may serve as the fundamental structure for more complicated energy storage systems.

REFERENCES

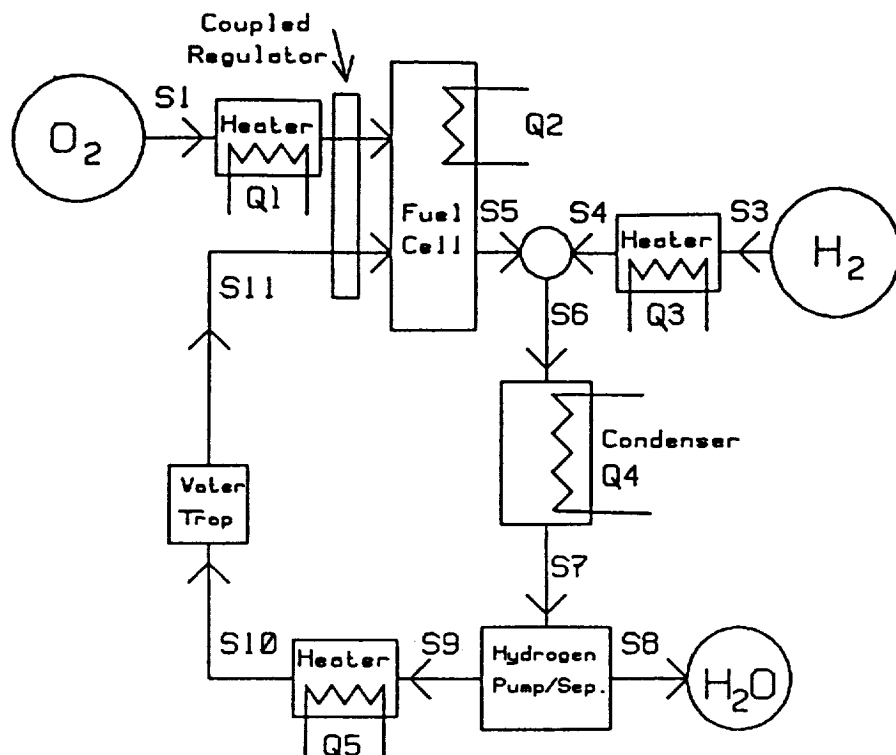
1. Leslie Van Dine, Olga Gonzalez-Sanabria, and Alexander Levy : "Regenerative Fuel Cell Study for Satellites in GEO Orbit", Proceedings of the 22nd Intersociety Energy Conversion Engineering Conference, Vol. 2, 1987, page 797.
2. Mark A. Hoberecht, Thomas B. Miller, Lorra L. Rieker, and Olga D. Gonzalez-Sanabria, "Design Considerations for a 10-kW Integrated Hydrogen-Oxygen Regenerative Fuel Cell System", 19th IECEC, 19-24 August, 1984.
3. Ralf Simon and Markus Rothmeyer : "Simulation of Regenerative Fuel Cell Systems Including Thermal Control", Proceedings of the European Space Power Conference, Madrid, Spain, 2-6 October, 1989, Volume 1, page 233.
4. McElroy, J.F., "SPE Regenerative Hydrogen/Oxygen Fuel Cells for Extraterrestrial Surface Applications, 24th IECEC, 6-11 August, 1989, Volume 3, page 1631.
5. David R. Saucier, "Hybrid Regenerative Fuel Cell Systems for Space Applications", 23rd IECEC, 7/31-8/5, 1988, Volume 2, page 291.
6. R.E. Martin. Final Report. Integrated Regenerative Fuel Cell Experimental Evaluation. NASA CR-185183.
7. P.A. Regenhardt, "F-CELL : The ASPEN Fuel Cell Model", U.S. Department of Energy, March 1985
8. Cheng-yi Lu, Internal NASA Communication.
9. K. Kordes, J.C.T. Oliveira, Ch. Gruber, and G. Winkler: "Water Removal Studies on High Power Hydrogen-Oxygen Fuel Cells with Alkaline Electrolytes", Proceedings of the European Space Power Conference, Madrid, Spain, 2-6 October, 1989, Volume 1, page 239.

TABLE I
Fuel Cell Operating Conditions

Operating Pressure	60 psia
Current Density	470 mA/sq.cm.
Active Area Per Cell	465 sq. cm.
Number of cells	132
Operation Time	344 hrs./cycle

TABLE II
Electrolyzer Operating Conditions

Operating Pressure	300 psia
Current Density	246.7 mA/sq.cm.
Active Area Per Cell	465 sq.cm.
Number of Cells	264
Operation Time	328 hrs./cycle



S1 : 0.269 kmol/hr O_2 ; 355 K
 S3 : 0.538 kmol/hr H_2
 S4 : 0.538 kmol/hr H_2 ; 355 K
 S5 : 5.979E-2 kmol/hr H_2
 0.538 kmol/hr H_2O ; 425 K
 S6 : 0.598 kmol/hr H_2
 0.538 kmol/hr H_2O ; 394 K
 S8 : 6.142E-8 kmol/hr H_2
 0.537 kmol/hr H_2O ; 280 K
 S9 : 0.598 kmol/hr H_2
 9.959E-4 kmol/hr H_2O ; 280 K
 S10: Temp.=355 K
 S11: 0.598 kmol/hr H_2 ; 355 K
 9.96E-6 kmol/hr H_2O

Q1 : Varies During Operation
 Q2 : -140.5 kcal/min
 Q3 : Varies During Operation
 Q4 : -118.3 kcal/min
 Q5 : 5.0 kcal/min

Power : 26.1 kW
 Voltage = 0.9 Volts/Cell
 Thermoneutral Voltage
 Efficiency : 71.9%

Figure 1. Flowsheet for Fuel Cell Subsection

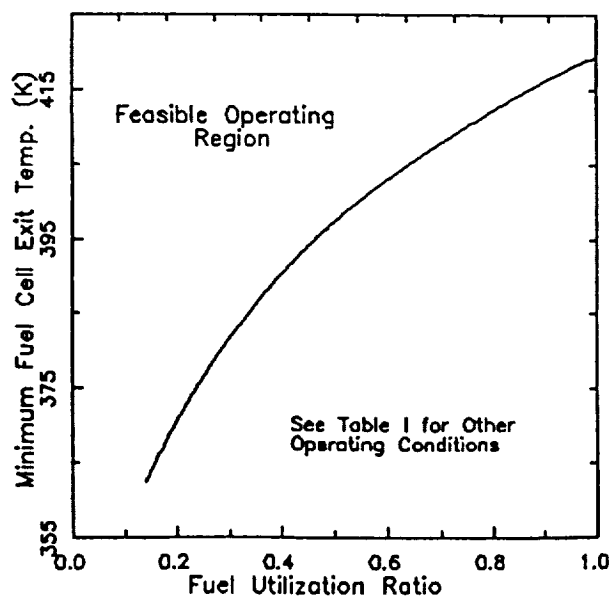


Figure 2. Relationship Between FUR and the Minimum Fuel Cell Exit Temperature

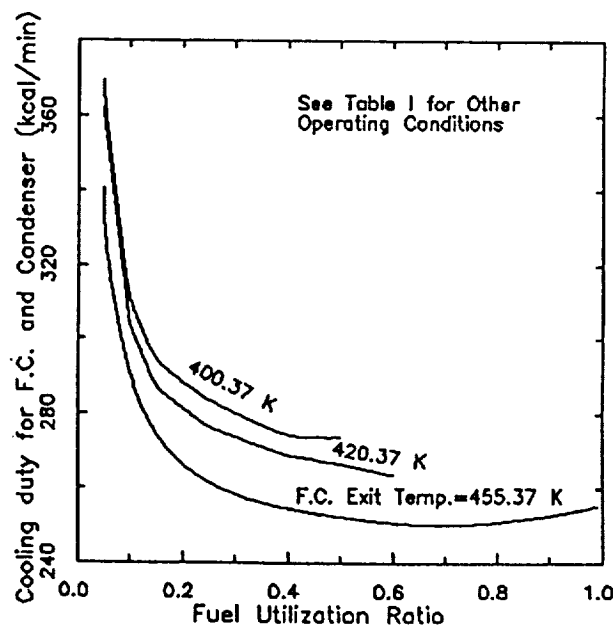
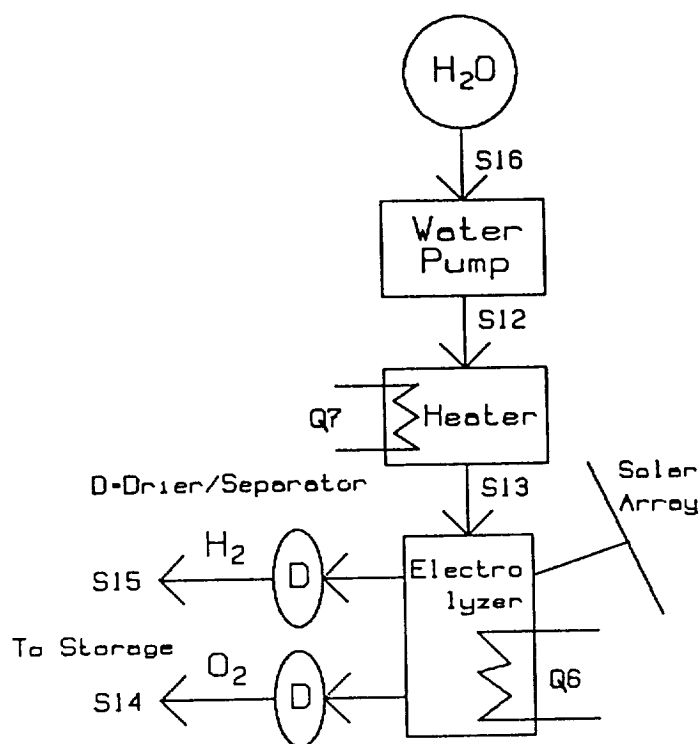


Figure 3. Effect of FUR on Fuel Cell and Condenser Cooling Requirements



S12: 0.565 kmol/hr H₂O
 6.45E-8 kmol/hr H₂
 S13: Temp. = 355.15 K
 S14: 0.282 kmol/hr O₂
 S15: 0.564 kmol/hr H₂
 S16: 0.565 kmol/hr H₂O
 6.45E-8 kmol/hr H₂

Q6 : 34.6 kcal/min
 Q7 : 13.8 kcal/min

Power Supplied : 42.9 kW
 Voltage = 1.4 Volts/Cell
 Thermoneutral Voltage
 Efficiency : 88.8%

Figure 4 Electrolyzer Subsection

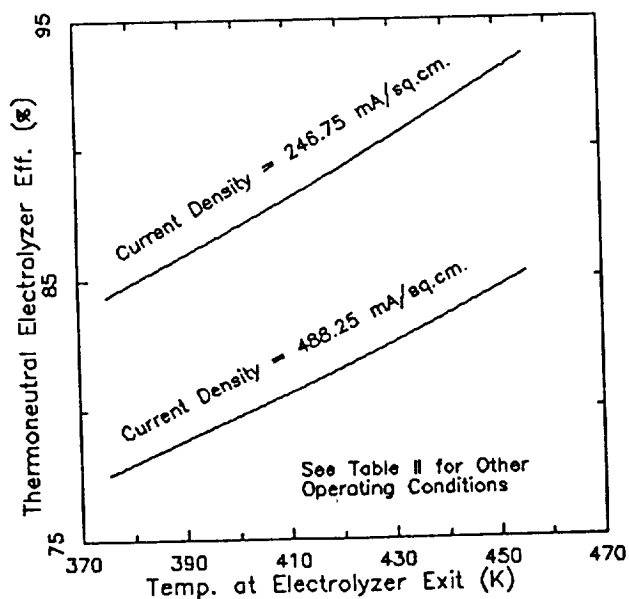


Figure 5. Relationship Between Electrolyzer Exit Temperature and Electrolyzer Efficiency

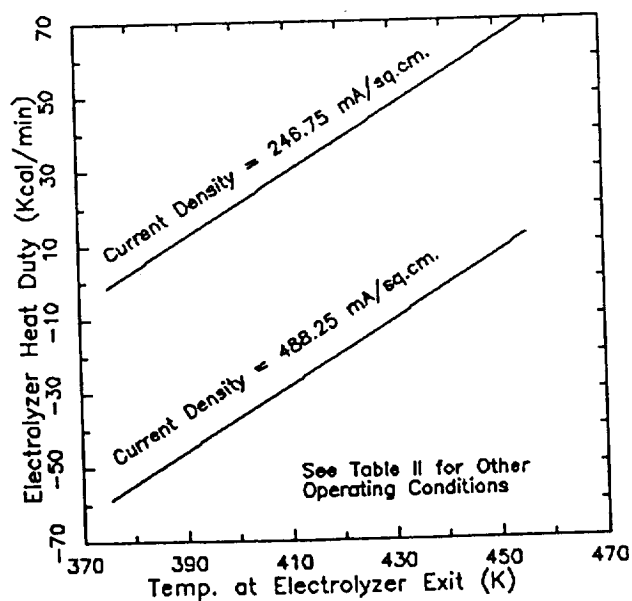


Figure 6. Relationship Between Electrolyzer Heat Duty and Electrolyzer Exit Temperature

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